

## Polarized entangled Bose-Einstein condensation

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We consider a mixture of two distinct species of atoms of pseudospin- $\frac{1}{2}$  with both intraspecies and interspecies spin-exchange interactions, and find all the ground states in a general case of the parameters in the effective Hamiltonian. In general, corresponding to the two species and two pseudo-spin states, there are four orbital wave functions into which the atoms condense. We find that in certain parameter regimes, the ground state is the so-called polarized entangled Bose-Einstein condensation, i.e. in addition to condensation of interspecies singlet pairs, there are unpaired atoms with spins polarized in the same direction. The interspecies entanglement and polarization significantly affect the generalized Gross-Pitaevskii equations governing the four orbital wave functions into which the atoms condense, as an interesting interplay between spin and orbital degrees of freedom.

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## I. INTRODUCTION

Since a decade ago, there have been a lot of activities on Bose-Einstein condensation (BEC) of atoms with spin degree of freedom [1], for example, in spin-1 [2–6] and pseudospin- $\frac{1}{2}$  gases [7–10], as well as BEC of a mixture of two kinds of spinless atoms [1, 11–17]. As a step beyond these research lines, a novel class of BEC, the so-called entangled BEC (EBEC), was proposed as the ground state of a mixture of two distinct species of pseudospin- $\frac{1}{2}$  atoms with interspecies spin exchange in some parameter regime [18–20]. Spin-exchange scattering between atoms of different species entangles these two species, and EBEC may lead to a novel kind of super-

fluidity [21]. More recently, EBEC has also been found in a mixture of spin-1 atoms [22]. It has been noted that EBEC may be experimentally realized using two different species of alkali atoms. In some aspects, EBEC bears some analogies with a single species of pseudospin- $\frac{1}{2}$  atoms in a double well [7] or occupying two orbital modes [8, 9], but there are also important differences due to the fact that two atoms of distinct species are distinguishable. In general, there are four orbital wave functions into which the atoms of the two species and two pseudospin states condense into, respectively.

Under single-mode approximation for orbital degree of freedom, the many-body Hamiltonian can be written as [19–21]

$$\mathcal{H} = \sum_{\alpha,\sigma} f_{\alpha\sigma} N_{i\sigma} + \frac{1}{2} \sum_{\alpha,\sigma\sigma'} K_{\sigma\sigma'}^{(\alpha\alpha)} N_{\alpha\sigma} N_{\alpha\sigma'} + \sum_{\sigma\sigma'} K_{\sigma\sigma'}^{(ab)} N_{a\sigma} N_{b\sigma'} + K_e (a_{\uparrow}^{\dagger} a_{\downarrow} b_{\downarrow}^{\dagger} b_{\uparrow} + a_{\downarrow}^{\dagger} a_{\uparrow} b_{\uparrow}^{\dagger} b_{\downarrow}), \quad (1)$$

where  $\alpha_{\sigma}$  ( $\alpha = a, b$ ,  $\sigma = \uparrow, \downarrow$ ) is the annihilation operator of the species  $\alpha$ ,

$$K_{\sigma\sigma'}^{(\alpha\beta)} \equiv g_{\sigma\sigma'}^{(\alpha\beta)} \int \phi_{\alpha\sigma}^*(\mathbf{r}) \phi_{\beta\sigma'}^*(\mathbf{r}) \phi_{\beta\sigma'}(\mathbf{r}) \phi_{\alpha\sigma}(\mathbf{r}) d^3r \quad (2)$$

is related to the scattering lengths as the following. In general,  $\xi_{\sigma_1\sigma_2\sigma_3\sigma_4}^{(\alpha\beta)}$  is the scattering length for the scattering in which an  $\alpha$ -atom flips from  $\sigma_4$  to  $\sigma_1$  while a  $\beta$ -atom flips from  $\sigma_3$  to  $\sigma_2$ ,  $\mu_{\alpha\beta} = m_{\alpha}m_{\beta}/(m_{\alpha} + m_{\beta})$  is the reduced mass. Now, for intraspecies scattering,  $g_{\sigma\sigma}^{(\alpha\alpha)} \equiv 2\pi\hbar^2 \xi_{\sigma\sigma\sigma\sigma}^{(\alpha\alpha)}/\mu_{\alpha\alpha}$  for same species and same spin,  $g_{\sigma\bar{\sigma}}^{(\alpha\alpha)} \equiv 4\pi\hbar^2 \xi_{\sigma\bar{\sigma}\sigma\bar{\sigma}}^{(\alpha\alpha)}/\mu_{\alpha\alpha} = 4\pi\hbar^2 \xi_{\sigma\bar{\sigma}\bar{\sigma}\sigma}^{(\alpha\alpha)}/\mu_{\alpha\alpha}$  for  $\sigma \neq \bar{\sigma}$ . For interspecies scattering without spin exchange,  $g_{\sigma\sigma'}^{(ab)} \equiv$

$2\pi\hbar^2 \xi_{\sigma\sigma'\sigma'\sigma}^{(ab)}/\mu_{\alpha\beta}$ , where  $\sigma$  and  $\sigma'$  may or may not be equal. For interspecies scattering with spin exchange,

$$K_e \equiv g_e \int \phi_{a\sigma}^*(\mathbf{r}) \phi_{b\bar{\sigma}}^*(\mathbf{r}) \phi_{b\sigma}(\mathbf{r}) \phi_{a\bar{\sigma}}(\mathbf{r}) d^3r, \quad (3)$$

where  $\sigma \neq \bar{\sigma}$ ,  $g_e \equiv g_{\sigma\bar{\sigma}\sigma\bar{\sigma}}^{(ab)} \equiv 2\pi\hbar^2 \xi_{\sigma\bar{\sigma}\sigma\bar{\sigma}}^{(ab)}/\mu_{\alpha\beta}$ .  $f_{\alpha\sigma} \equiv \epsilon_{\alpha\sigma} - K_{\sigma\sigma}^{(\alpha\alpha)}/2$ , where  $\epsilon_{\alpha\sigma} = \int \phi_{\alpha\sigma}^* h_{\alpha\sigma} \phi_{\alpha\sigma} d^3r$  is the single-particle energy,  $h_{\alpha\sigma}$  being the single-particle Hamiltonian.

The total spin operator of species  $\alpha$  ( $\alpha = a, b$ ) is  $\mathbf{S}_{\alpha} = \alpha_{\sigma}^{\dagger} \mathbf{s}_{\sigma\sigma'} \alpha'_{\sigma}$ , where  $\mathbf{s}_{\sigma\sigma'}$  is the single spin operator. Hence the Hamiltonian can be transformed into that of two coupled giant spins,

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$$\mathcal{H} = 2K_e(S_{ax}S_{bx} + S_{ay}S_{by}) + J_z S_{az}S_{bz} + B_a S_{az} + B_b S_{bz} + C_a S_{az}^2 + C_b S_{bz}^2 + E_0, \quad (4)$$

where  $J_z = K_{\uparrow\uparrow}^{(ab)} + K_{\downarrow\downarrow}^{(ab)} - K_{\uparrow\downarrow}^{(ab)} - K_{\downarrow\uparrow}^{(ab)}$ ,  $B_a = f_{a\uparrow} - f_{a\downarrow} + \frac{N_a}{2}(K_{\uparrow\uparrow}^{(aa)} - K_{\downarrow\downarrow}^{(aa)}) + \frac{N_b}{2}(K_{\uparrow\uparrow}^{(ab)} + K_{\uparrow\downarrow}^{(ab)} - K_{\downarrow\uparrow}^{(ab)} - K_{\downarrow\downarrow}^{(ab)})$ ,  $B_b = f_{b\uparrow} - f_{b\downarrow} + \frac{N_b}{2}(K_{\uparrow\uparrow}^{(bb)} - K_{\downarrow\downarrow}^{(bb)}) + \frac{N_a}{2}(K_{\uparrow\uparrow}^{(ab)} + K_{\uparrow\downarrow}^{(ab)} - K_{\downarrow\uparrow}^{(ab)} - K_{\downarrow\downarrow}^{(ab)})$ ,  $C_a = \frac{1}{2}(K_{\uparrow\uparrow}^{(aa)} + K_{\downarrow\downarrow}^{(aa)} - K_{\uparrow\downarrow}^{(aa)} - K_{\downarrow\uparrow}^{(aa)})$ ,  $C_b = \frac{1}{2}(K_{\uparrow\uparrow}^{(bb)} + K_{\downarrow\downarrow}^{(bb)} - K_{\uparrow\downarrow}^{(bb)} - K_{\downarrow\uparrow}^{(bb)})$ .  $E_0 = (1/2)\sum_{\alpha}(\sum_{\sigma} f_{\alpha\sigma})N_{\alpha} + (1/8)\sum_{\alpha}(\sum_{\sigma\sigma'} K_{\sigma\sigma'}^{(\alpha\alpha)})N_{\alpha}^2 + (1/4)(\sum_{\sigma\sigma'} K_{\sigma\sigma'}^{(ab)})N_a N_b$  does not depend on spins. We label the two species in such a way that  $N_a \geq N_b$ .

As discussed previously, at the antiferromagnetic isotropic point of the effective parameters, namely  $2K_e = J_z > 0$  while  $B_a = B_b = C_a = C_b = 0$ ,  $\mathcal{H} = 2K_e \mathbf{S}_a \cdot \mathbf{S}_b$ . Then the ground states are  $|\frac{N_a - N_b}{2}, S_z\rangle = Z(a_{\uparrow}^{\dagger})^{N_a/2 - N_b/2 + S_z} (a_{\downarrow}^{\dagger})^{N_a/2 - N_b/2 - S_z} (a_{\uparrow}^{\dagger} b_{\downarrow}^{\dagger} - a_{\downarrow}^{\dagger} b_{\uparrow}^{\dagger})^{N_b} |0\rangle$ , where  $Z$  is the normalization constant. This ground state leads to interesting physical consequences. It has been shown numerically and analytically that EBEC also persists in a considerable regime away from the isotropic point.

In this paper, we extend the consideration of this model to a more general case of the parameters, namely,  $B_a = B_b$ , denoted as  $B$ ,  $C_a = C_b$ , denoted as  $C$ , and  $J_z - 2K_e - 2C = 0$ , and thus the Hamiltonian becomes

$$\mathcal{H} = 2K_e \mathbf{S}_a \cdot \mathbf{S}_b + B S_z + C S_z^2 + E_0. \quad (5)$$

which reduces to the isotropic antiferromagnetic coupling when  $B = C = 0$  while  $K_e > 0$ . In other words, we assume that there is such a rotational symmetry that the Hamiltonian only depends on the total  $S$  and  $S_z$ , which are thus good quantum numbers. We believe that under a perturbation due to deviation of the parameters from this condition, the ground state is still close to the present one in each parameter regime discussed below, based on an extension of the previous analysis for the isotropic parameter point [20], the details of which will be reported elsewhere.

In Sec. II, we find all the ground states of the Hamiltonian (5) in various parameter regimes, based on the calculation accounted in the Appendices. In Sec. III, these ground states are expressed in terms of Bosonic degrees of freedom. Most of the ground states are of the form of  $|S, \pm S\rangle$ , which are referred to as the polarized BEC if  $S \neq 0$ , as then  $S_z = \pm S \neq 0$ . Their properties are discussed in Sec. IV. A summary is given in Sec. V.

## II. GROUND STATES IN VARIOUS PARAMETER REGIMES

For spin- $\frac{1}{2}$  atoms,  $S_a = N_a/2$  and  $S_b = N_b/2$  are fixed. It is clear that the total spin  $S$  and its  $z$ -component  $S_z$  are good quantum numbers, hence the eigenstates are of

the form of  $|S, S_z\rangle$ . The ground state is thus

$$|G\rangle = |S^m, S_z^m\rangle, \quad (6)$$

where  $S^m$  and  $S_z^m$  are, respectively, the values of  $S$  and  $S_z$  that minimize

$$E = K_e S(S+1) + B S_z + C S_z^2 \quad (7)$$

In case  $C \neq 0$ , it can be rewritten as

$$E = K_e \left(S + \frac{1}{2}\right)^2 + C \left(S_z + \frac{B}{2C}\right)^2 + E'_0, \quad (8)$$

where  $E'_0$  is independent of  $S$  and  $S_z$ . The minimization should be under the constraints

$$S_{min} \leq S \leq S_{max}, \quad (9)$$

$$-S \leq S_z \leq S, \quad (10)$$

where

$$S_{min} \equiv S_a - S_b = \frac{N_a - N_b}{2}, \quad (11)$$

$$S_{max} \equiv S_a + S_b = \frac{N_a + N_b}{2}. \quad (12)$$

We have obtained all the ground states in the whole three-dimensional  $C - K_e - B$  parameter space.

### A. $B \neq 0$

Based on the calculations in Appendix A, the ground states for  $B \neq 0$  are summarized in Table I, and in the two-dimensional  $C - K_e$  phase diagrams for a given  $B \neq 0$ , as shown in FIG. 1, as well as FIG. 2 for the special case of  $N_a = N_b = N$ .

In the regime  $K_e < \frac{|B| - N_a C}{N_a + 1}$  for  $C < -|B|$  plus  $K_e \leq \frac{|B| - (N_a + N_b)C}{N_a + N_b + 1}$  for  $-|B| < C \leq \frac{|B|}{N_a + N_b}$ , the ground state is  $|\frac{N_a + N_b}{2}, -\text{sgn}(B)(\frac{N_a + N_b}{2})\rangle$ , where  $\text{sgn}(B)$  denotes the sign of  $B$ .

In the regime  $K_e > \frac{|B| - N_a C}{N_a + 1}$  for  $C < -|B|$  plus  $K_e \geq \frac{|B| - (N_a - N_b)C}{N_a - N_b + 1}$  for  $-|B| < C \leq \frac{|B|}{N_a - N_b}$ , the ground state is  $|\frac{N_a - N_b}{2}, -\text{sgn}(B)(\frac{N_a - N_b}{2})\rangle$ . Note that if  $N_a = N_b$ , then this statement is still valid by regarding  $\frac{|B|}{N_a - N_b}$  as infinity. In other words, the boundary  $C = \frac{|B|}{N_a - N_b}$  disappears, and the ground state is  $|0, 0\rangle$  in the whole regime of  $K_e > \frac{|B| - N_a C}{N_a + 1}$  for  $C < -|B|$  plus  $K_e \geq |B|$  for  $C > -|B|$ .

On the boundary  $K_e = \frac{|B| - N_a C}{N_a + 1}$  for  $C < -|B|$ ,  $|\frac{N_a + N_b}{2}, -\text{sgn}(B)(\frac{N_a + N_b}{2})\rangle$  and

Parameter regimes			Ground states $ S^m, S_z^m\rangle$
$B \neq 0$	$C < - B $	$K_e < \frac{ B -N_a C}{N_a+1}$	$ \frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$
		$K_e = \frac{ B -N_a C}{N_a+1}$	$ \frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$ and $ \frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$
		$K_e > \frac{ B -N_a C}{N_a+1}$	$ \frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$
	$C = - B $	$K_e < -C$	$ \frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$
		$K_e = -C$	$ S^m, -\text{sgn}(B)S^m\rangle, \frac{N_a-N_b}{2} \leq S^m \leq \frac{N_a+N_b}{2}$
		$K_e > -C$	$ \frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$
	$- B  < C \leq \frac{ B }{N_a+N_b}$	$K_e \leq \frac{ B -(N_a+N_b)C}{N_a+N_b+1}$	$ \frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$
		$\frac{ B -(N_a+N_b)C}{N_a+N_b+1} \leq K_e \leq \frac{ B -(N_a-N_b)C}{N_a-N_b+1}$	$ s, -\text{sgn}(B)s\rangle, s = \text{Int}(\frac{ B -K_e}{2(K_e+C)})$
		$K_e \geq \frac{ B -(N_a+N_b)C}{N_a+N_b+1}$	$ \frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$
	$\frac{ B }{N_a+N_b} \leq C \leq \frac{ B }{N_a-N_b}$	$K_e < 0$	$ \frac{N_a+N_b}{2}, \text{Int}(-\frac{B}{2C})\rangle$
		$K_e = 0$	$ S^m, \text{Int}(-\frac{B}{2C})\rangle,  \text{Int}(-\frac{B}{2C})  \leq S^m \leq \frac{N_a+N_b}{2}$
		$0 < K_e \leq \frac{ B -(N_a-N_b)C}{N_a-N_b+1}$	$ s, -\text{sgn}(B)s\rangle, s = \text{Int}(\frac{ B -K_e}{2(K_e+C)})$
		$K_e \geq \frac{ B -(N_a-N_b)C}{N_a-N_b+1}$	$ \frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$
	$C \geq \frac{ B }{N_a-N_b}$	$K_e < 0$	$ \frac{N_a+N_b}{2}, \text{Int}(-\frac{B}{2C})\rangle$
		$K_e = 0$	$ S^m, \text{Int}(-\frac{B}{2C})\rangle,  \text{Int}(-\frac{B}{2C})  \leq S^m \leq \frac{N_a+N_b}{2}$
		$K_e > 0$	$ \frac{N_a-N_b}{2}, \text{Int}(-\frac{B}{2C})\rangle$

TABLE I. Ground states in various parameter regimes with  $B \neq 0$ .

$|\frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$  are the two degenerate ground states.

In the regime  $\frac{|B|-(N_a+N_b)C}{N_a+N_b+1} \leq K_e \leq \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$  and  $K_e > 0$  for  $-|B| < C \leq \frac{|B|}{N_a-N_b}$ , the ground state is  $|s, -\text{sgn}(B)s\rangle$ , where  $s \equiv \text{Int}(S_0)$  is the integer closest to  $S_0 \equiv \frac{|B|-K_e}{2(K_e+C)}$  and in the legitimate range  $S_{\min} \leq s \leq S_{\max}$ . When  $N_a = N_b$ , the boundary  $K_e = \frac{|B|-(N_a+N_b)C}{N_a+N_b+1}$  becomes  $K_e = |B|$  for  $C > -|B|$  up to infinity. This is a crossover regime, as  $s$  depends on the parameters, and is continuously connected with the two neighboring regimes, that is,  $s = \frac{N_a+N_b}{2}$  at the boundary  $K_e = \frac{|B|-(N_a+N_b)C}{N_a+N_b+1}$  while  $s = \frac{N_a-N_b}{2}$  at the boundary  $K_e = \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$ . But there are discontinuities on the boundary  $K_e = 0$  for  $\frac{|B|}{N_a+N_b} \leq C \leq \frac{|B|}{N_a-N_b}$ .

In the regime  $C \geq \frac{|B|}{N_a+N_b}$  while  $K_e < 0$ , the ground state is  $|\frac{N_a+N_b}{2}, -\text{Int}(\frac{B}{2C})\rangle$ . It is continuously connected with  $|\frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$  on the boundary  $C = \frac{|B|}{N_a+N_b}$  while  $K_e \leq 0$ .

Finally, for  $N_a > N_b$ , in the regime  $C \geq \frac{|B|}{N_a-N_b}$  while  $K_e > 0$ , the ground state is  $|\frac{N_a-N_b}{2}, \text{Int}(-\frac{B}{2C})\rangle$ . It is continuously connected with  $|\frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$  on the boundary  $C = \frac{|B|}{N_a-N_b}$  while  $K_e > 0$ .

On the boundary  $K_e = 0$  while  $\frac{|B|}{N_a+N_b} \leq C \leq \frac{|B|}{N_a-N_b}$ , the degenerate ground states are  $|S^m, \text{Int}(-\frac{B}{2C})\rangle$ , with  $|\text{Int}(-\frac{B}{2C})| \leq S^m \leq \frac{N_a+N_b}{2}$ . On the boundary  $K_e = 0$  while  $C \geq \frac{|B|}{N_a-N_b}$ , the degenerate ground states are  $|S^m, \text{Int}(-\frac{B}{2C})\rangle$ , with  $\frac{N_a-N_b}{2} \leq S^m \leq \frac{N_a+N_b}{2}$ . The ground state in each regime bordering each of these two

boundaries is one of the ground states on it. Hence discontinuities or quantum phase transitions occur in crossing this boundary from one regime to another.

The only other boundary where discontinuity or quantum phase transitions occur is  $K_e = \frac{|B|-N_a C}{N_a+1}$  for  $C < -|B|$ . In entering it from downside or upside, the ground state remains as the original one, but when leaving it and entering the other side, the ground state discontinuously changes to another state. Nevertheless, if entering the boundary from the crossover regime  $\frac{|B|-(N_a+N_b)C}{N_a+N_b+1} \leq K_e \leq \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$  and  $K_e > 0$  for  $-|B| < C \leq \frac{|B|}{N_a-N_b}$ , there is no discontinuity, as the ground state  $|s, -\text{sgn}(B)s\rangle$  in this regime is continuously connected with both  $|\frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$  and  $|\frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$ .

Three boundaries  $K_e = \frac{|B|-N_a C}{N_a+1}$  for  $C < -|B|$ ,  $K_e = \frac{|B|-(N_a+N_b)C}{N_a+N_b+1}$  and  $K_e = \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$  for  $C > -|B|$  converge at  $K_e = -C = |B|$ , which does not belong to any of these three regimes and where the ground state can be any state  $|S^m, S_z^m\rangle$ , with  $S^m$  and  $S_z^m$  in the legitimate ranges, or any superposition of these states. In the three dimensional  $C - K_e - B$  parameter space, these three boundaries that are lines on the  $C - K_e$  plane with a given  $B$  become planes.  $K_e = -C = |B|$  are two lines converging at the origin for  $B \geq 0$  and  $B \leq 0$  respectively.

The structure of the three-dimensional phase diagram possesses a reflection symmetry with respect to the plane  $B = 0$ . In each pair of symmetric regimes, the ground states have the same  $S^m$  but opposite  $S_z^m$ .

As  $B \rightarrow 0$ , the boundary  $C = \frac{|B|}{N_a+N_b}$  for  $K_e \leq 0$  ap-

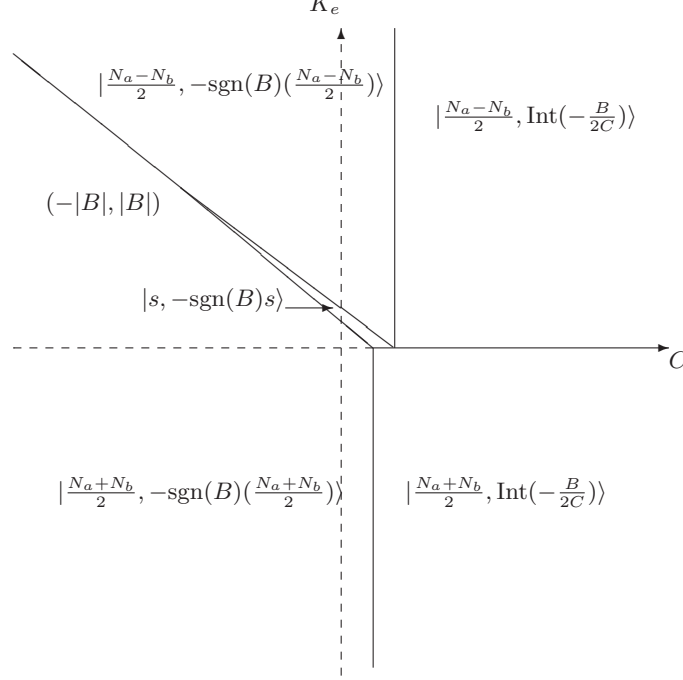


FIG. 1. Ground states in  $C - K_e$  parameter plane for a given  $B \neq 0$ , which can be positive or negative. The solid lines are boundaries between different regimes. The dashed lines are only coordinate axes. The ground states in five regimes are indicated.  $|s, -\text{sgn}(B)s\rangle$ , with  $s \equiv \text{Int}(\frac{|B|-K_e}{2(K_e+C)})$ , is the ground state in the regime surrounded by  $K_e = \frac{|B|-(N_a+N_b)C}{N_a+N_b+1}$ ,  $K_e = \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$  and  $K_e = 0$ , which is continuously connected with  $|\frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$  and  $|\frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$  on the two boundaries, respectively. The boundary for  $C < -|B|$  is  $K_e = \frac{|B|-N_a C}{N_a+1}$ , on which both  $|\frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$  and  $|\frac{N_a-N_b}{2}, -\text{sgn}(B)(\frac{N_a-N_b}{2})\rangle$  are degenerate ground states. Three boundary lines converge at  $K_e = -C = |B|$ , on which any state is the ground state. The ground state  $|\frac{N_a+N_b}{2}, -\text{Int}(\frac{B}{2C})\rangle$  is continuously connected with  $|\frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$  on the boundary  $C = \frac{|B|}{N_a+N_b}$  while  $K_e < 0$ .  $|\frac{N_a-N_b}{2}, \text{Int}(-\frac{B}{2C})\rangle$  is continuously connected with  $|\frac{N_a+N_b}{2}, -\text{sgn}(B)(\frac{N_a+N_b}{2})\rangle$  on the boundary  $C = \frac{|B|}{N_a-N_b}$  while  $K_e > 0$ . On the boundary  $K_e = 0$  while  $\frac{|B|}{N_a+N_b} \leq C \leq \frac{|B|}{N_a-N_b}$ , the degenerate ground states are of the form of  $|S^m, \text{Int}(-\frac{B}{2C})\rangle$  with  $|\text{Int}(-\frac{B}{2C})| \leq S^m \leq \frac{N_a+N_b}{2}$ . On the boundary  $K_e = 0$  while  $C \geq \frac{|B|}{N_a-N_b}$ , the degenerate ground states are of the form of  $|S^m, \text{Int}(-\frac{B}{2C})\rangle$  with  $\frac{N_a-N_b}{2} \leq S^m \leq \frac{N_a+N_b}{2}$ . This figure reduces to FIG. 2 in the special case of  $N_a = N_b$ .

proaches the negative half of  $K_e$ -axis including the origin, while the boundary  $C = \frac{|B|}{N_a-N_b}$  for  $K_e > 0$ , existing when  $N_a > N_b$ , approaches the positive half of  $K_e$ -axis excluding the origin. The boundary  $K_e = \frac{|B|-N_a C}{N_a+1}$  for  $C < -|B|$  approaches  $K_e = \frac{-N_a C}{N_a+1}$  for  $C < 0$ , while the crossover regime of  $|s, -\text{sgn}(B)s\rangle$  tends to vanish, and  $K_e = -C = |B|$  approaches the origin  $K_e = -C = |B| = 0$ .

### B. $B = 0$

Based on the calculations in Appendix B, the ground states for  $B = 0$  are summarized in Table II, and depicted in the two-dimensional  $C - K_e$  phase diagrams for  $B = 0$ , as shown in FIG. 3.

For  $C > 0$ ,  $K_e > 0$  while  $B = 0$ , the ground state

is uniquely  $|\frac{N_a-N_b}{2}, 0\rangle$ . In the case of  $N_a > N_b$ , it is continuously connected with  $|\frac{N_a-N_b}{2}, \text{Int}(-\frac{B}{2C})\rangle$  in the regime  $C > \frac{|B|}{N_a-N_b}$ ,  $K_e > 0$  while  $B \neq 0$ . In the case of  $N_a = N_b$ , the ground state for  $C > 0$ ,  $K_e > 0$  while  $B = 0$  becomes  $|0, 0\rangle$ , which is the same one as for  $C > 0$  while  $K_e > |B|$ .

For  $C > 0$ ,  $K_e < 0$  while  $B = 0$ , the ground state is uniquely  $|\frac{N_a+N_b}{2}, 0\rangle$ . It is continuously connected with  $|\frac{N_a+N_b}{2}, -\text{Int}(\frac{B}{2C})\rangle$  in the regime  $C > \frac{|B|}{N_a+N_b}$ ,  $K_e < 0$  while  $B \neq 0$ .

On the boundary  $C > 0$ ,  $K_e = 0$  while  $B = 0$ , i.e. on the positive  $C$  axis, the degenerate ground states are  $|S^m, 0\rangle$ , with  $\frac{N_a-N_b}{2} \leq S^m \leq \frac{N_a+N_b}{2}$ , which include the two ground states in the regimes above and below this half axis. In case  $N_a > N_b$ , these degenerate ground states on positive  $C$  axis is continuously connected with  $|S^m, \text{Int}(-\frac{B}{2C})\rangle$ , with  $\frac{N_a-N_b}{2} \leq S^m \leq \frac{N_a+N_b}{2}$ , on the

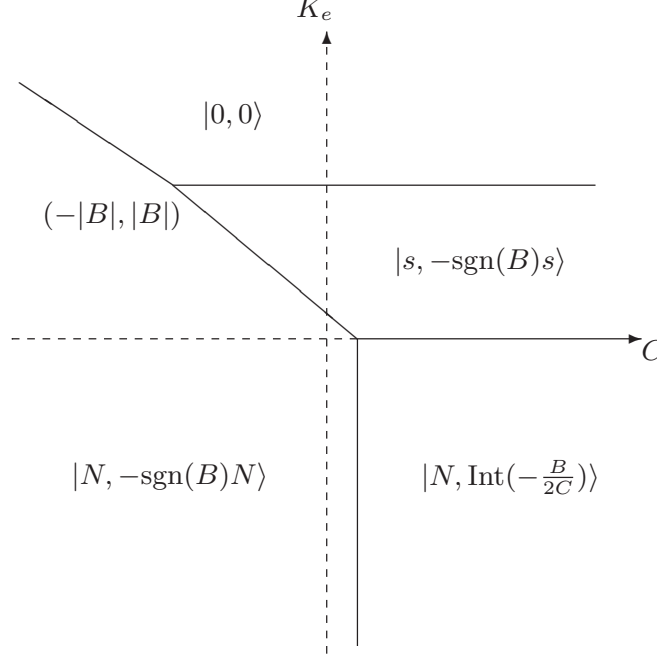


FIG. 2. Ground states in  $C - K_e$  parameter plane for a given  $B \neq 0$  in the special case of  $N_a = N_b = N$ . This diagram is a limit of FIG. 1, with the boundary  $C = \frac{|B|}{N_a - N_b}$  disappearing while the boundary  $K_e = \frac{|B| - (N_a - N_b)C}{N_a - N_b + 1}$  becoming a horizontal line  $K_e = |B|$ .

Parameter regimes			Ground states $ S^m, S_z^m\rangle$
$B = 0$	$C > 0$	$K_e > 0$	$ \frac{N_a - N_b}{2}, 0\rangle$
		$K_e = 0$	$ S^m, 0\rangle, \frac{N_a - N_b}{2} \leq S^m \leq \frac{N_a + N_b}{2}$
		$K_e < 0$	$ \frac{N_a + N_b}{2}, 0\rangle$
	$C = 0$	$K_e > 0$	$ \frac{N_a - N_b}{2}, S_z^m\rangle, -\frac{N_a - N_b}{2} \leq S_z^m \leq \frac{N_a - N_b}{2}$
		$K_e = 0$	$ S^m, S_z^m\rangle, \frac{N_a - N_b}{2} \leq S^m \leq \frac{N_a + N_b}{2}, -S^m \leq S_z^m \leq S^m$
		$K_e < 0$	$ \frac{N_a + N_b}{2}, S_z^m\rangle, -\frac{N_a + N_b}{2} \leq S_z^m \leq \frac{N_a + N_b}{2}$
	$C < 0$	$K_e > -\frac{N_a C}{N_a + 1}$	$ \frac{N_a - N_b}{2}, \pm \frac{N_a - N_b}{2}\rangle$
		$K_e = -\frac{N_a C}{N_a + 1}$	$ \frac{N_a - N_b}{2}, \pm \frac{N_a - N_b}{2}\rangle$ and $ \frac{N_a + N_b}{2}, \pm \frac{N_a + N_b}{2}\rangle$
		$K_e < -\frac{N_a C}{N_a + 1}$	$ \frac{N_a + N_b}{2}, \pm \frac{N_a + N_b}{2}\rangle$

TABLE II. Ground states in various parameter regimes with  $B = 0$ .

boundary  $K_e = 0$ ,  $C \geq \frac{|B|}{N_a - N_b}$  while  $B \neq 0$ . In case  $N_a = N_b$ , these ground states are continuously connected with the ground states  $|S^m, \text{Int}(-\frac{B}{2C})\rangle$ , with  $\text{Int}(-\frac{B}{2C}) \leq S^m \leq \frac{N_a + N_b}{2}$ , on the boundary  $K_e = 0$ ,  $C \geq \frac{|B|}{N_a + N_b}$  while  $B \neq 0$ .

For  $C < 0$ ,  $K_e > -\frac{N_a C}{N_a + 1}$  while  $B = 0$ , the twofold degenerate ground states are  $|\frac{N_a - N_b}{2}, \pm \frac{N_a - N_b}{2}\rangle$ . Similarly, for  $C < 0$ ,  $K_e < -\frac{N_a C}{N_a + 1}$  while  $B = 0$ , the twofold degenerate ground states are  $|\frac{N_a + N_b}{2}, \pm \frac{N_a + N_b}{2}\rangle$ . On the boundary  $C < 0$ ,  $K_e = -\frac{N_a C}{N_a + 1}$  while  $B = 0$ , the fourfold degenerate ground states are  $|\frac{N_a - N_b}{2}, \pm \frac{N_a - N_b}{2}\rangle$  and

$|\frac{N_a + N_b}{2}, \pm \frac{N_a + N_b}{2}\rangle$ , just the union of the ground states above and below this axis.

For  $B = 0$ , on  $K_e$  axis, the ground states are always degenerate too. For  $C = 0$ ,  $K_e > 0$  while  $B = 0$ , i.e. on the positive  $K_e$  axis, the ground states are  $|\frac{N_a - N_b}{2}, S_z^m\rangle$ , with  $-\frac{N_a - N_b}{2} \leq S_z^m \leq \frac{N_a - N_b}{2}$ , which include the ground states in the regimes on the right and left of this half axis. This is the ground states discussed previously. For  $B = 0$ ,  $C = 0$  while  $K_e < 0$ , i.e. on the negative  $K_e$  axis, the ground states are  $|\frac{N_a + N_b}{2}, S_z^m\rangle$ , with  $-\frac{N_a + N_b}{2} \leq S_z^m \leq \frac{N_a + N_b}{2}$ , which, again, include the ground states in the regimes on the right and left of this half axis.

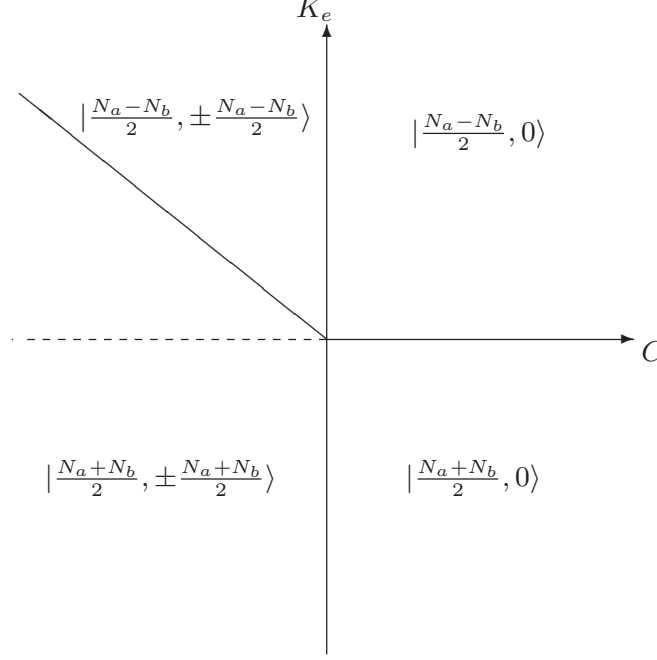


FIG. 3. Ground states in  $C - K_e$  parameter plane for  $B = 0$ . The solid lines are boundaries between different regimes. The dashed line is only the negative  $C$  axis. The ground states in four regimes are indicated. The boundary for  $C < 0$  is  $K_e = -\frac{N_a C}{N_a + 1}$ , on which both  $|\frac{N_a + N_b}{2}, \pm \frac{N_a + N_b}{2}\rangle$  and  $|\frac{N_a - N_b}{2}, \pm \frac{N_a - N_b}{2}\rangle$  are degenerate ground states. On the positive  $C$  axis, the ground states are  $|S^m, 0\rangle$ , with  $\frac{N_a - N_b}{2} \leq S^m \leq \frac{N_a + N_b}{2}$ . On the positive  $K_e$  axis, the ground states are  $|\frac{N_a - N_b}{2}, S_z^m\rangle$ , with  $-\frac{N_a - N_b}{2} \leq S_z^m \leq \frac{N_a - N_b}{2}$ . On the negative  $K_e$  axis, the ground states are  $|\frac{N_a + N_b}{2}, S_z^m\rangle$ , with  $-\frac{N_a + N_b}{2} \leq S_z^m \leq \frac{N_a + N_b}{2}$ . On the origin  $B = C = K_e = 0$ , the ground state can be any superposition of  $|S^m, S_z^m\rangle$ , with  $\frac{N_a - N_b}{2} \leq S^m \leq \frac{N_a + N_b}{2}$  and  $-S^m \leq S_z^m \leq S^m$ .

At the origin  $B = C = K_e = 0$ , the ground state can be any legitimate state, i.e.  $|S^m, S_z^m\rangle$ , with  $\frac{N_a - N_b}{2} \leq S^m \leq \frac{N_a + N_b}{2}$  and  $-S^m \leq S_z^m \leq S^m$ , or any of their superposition.

Therefore in the case of  $B = 0$ , all the boundaries on  $C - K_e$  parameter plane is a phase boundary, on which discontinuities or quantum phase transitions occur. The degenerate ground states on the boundary include the ones in the regimes it divides.

As  $B \rightarrow 0$ , the boundaries of different  $C - K_e$  regime for  $B \neq 0$  converge to those of  $B = 0$ . A ground state in each  $C - K_e$  regime on each side of  $B = 0$  reduces to a ground state in the corresponding  $C - K_e$  regime for  $B = 0$ . For  $C > 0$ , all the ground states for  $B \neq 0$  are continuously connected with those for  $B = 0$ . For  $B = 0$  while  $K_e \leq 0$ , the ground states in the regime  $C > 0$  can be obtained by substituting  $B = 0$  in the ground state for  $C > \frac{|B|}{N_a + N_b}$  while  $K_e \leq 0$ . For  $B = 0$  while  $K_e > 0$ , the ground states in the regime  $C > 0$  can be obtained by substituting  $B = 0$  in the ground state for  $C > \frac{|B|}{N_a - N_b}$  while  $K_e > 0$  in case  $N_a > N_b$ , and it is the same as the ground state for  $C > 0$  while  $K_e > |B|$  in case  $N_a = N_b$ .

For  $C \leq 0$  while  $B = 0$ , excluding the origin  $B = C = K_e = 0$ , the ground states in each  $C - K_e$  regime include ground states on both sides of  $B = 0$ . Hence for  $C \leq 0$ , there is always a discontinuity or quantum phase transition in the ground state when  $B$  switches its sign from positive to negative and vice versa, for any values of  $K_e$ . When  $B$  continuously reduce the magnitude, the ground state remains as the initial one when reaching  $B = 0$ , then the discontinuity in ground state occurs when the sign  $B$  becomes opposite to the original.

### III. GROUND STATES IN TERMS OF BOSON OPERATORS

One can obtain the expression of any ground state  $|S, S_z\rangle$  in terms of bosonic degrees of freedom, using

$$|S, S_z\rangle = \sum_{S_{bz}=-S_b}^{S_b} g(S, S_z, S_{bz}) |S_a, S_z - S_{bz}\rangle_a |S_b, S_{bz}\rangle_b, \quad (13)$$

where  $g(S, S_z, S_{bz}) \equiv \langle S_a, S_z - S_{bz}, S_b, S_{bz} | S, -S \rangle$  is the Clebsch-Gordan coefficient [23]

$$\begin{aligned}
g(S, S_z, S_{bz}) &= \langle S_a, S_z - S_{bz}; S_b, S_{bz} | S_a, S_b, S, S_z \rangle = \left[ \frac{(2S+1)(S_a + S_b - S)!(S_a - S_b + S)!(S_b - S_a + S)!}{(S_a + S_b + S + 1)!} \right]^{\frac{1}{2}} \\
&\times [(S_a + S_z - S_{bz})!(S_a - S_z + S_{bz})!(S_b + S_{bz})!(S_b - S_{bz})!(S + S_z)!(S - S_z)!]^{\frac{1}{2}} \\
&\times \sum_k (-1)^k [k!(S_a + S_b - S - k)!(S_a - S_z + S_{bz} - k)!(S_b + S_{bz} - k)!(S - S_b + S_z - S_{bz} + k)!(S - S_a - S_{bz} + k)!]^{-1},
\end{aligned} \tag{14}$$

where  $k$  is an integer such that the arguments in the factorials are non-negative. In terms of the particle number in each single particle mode  $\alpha = a, b$ ,

$$|S_\alpha, S_{\alpha z}\rangle_\alpha = |S_\alpha + S_{\alpha z}\rangle_{\alpha\uparrow} |S_\alpha - S_{\alpha z}\rangle_{\alpha\downarrow}, \tag{15}$$

where  $|n\rangle_{\alpha\sigma} = \frac{1}{\sqrt{n!}}(\alpha_\sigma^\dagger)^n|0\rangle$ , ( $\sigma = \uparrow, \downarrow$ ).

Therefore,

$$|S, S_z\rangle = \sum_{S_{bz}=-S_b}^{S_b} f(S, S_z, S_{bz})(a_\uparrow^\dagger)^{S_a+S_z-S_{bz}}(a_\downarrow^\dagger)^{S_a-S_z+S_{bz}}(b_\uparrow^\dagger)^{S_b+S_{bz}}(b_\downarrow^\dagger)^{S_b-S_{bz}}|0\rangle, \tag{16}$$

with

$$f(S, S_z, S_{bz}) = g(S, S_z, S_{bz})[(S_a + S_z - S_{bz})!(S_a - S_z + S_{bz})!(S_b + S_{bz})!(S_b - S_{bz})!]^{-1/2}.$$

In some special cases, to which most of our ground states belong, this expression can be simplified as the following.

#### A. $|S, \pm S\rangle$

For  $S_z = -S$ , we have

$$g(S, -S, S_{bz}) = (-1)^{S_b+S_{bz}} \left[ \frac{(2S+1)!(S_a + S_b - S)!(S_a + S_{bz} + S)!(S_b - S_{bz})!}{(S_a + S_b + S + 1)!(S_a - S_b + S)!(S_a - S - S_{bz})!(S_b + S_{bz})!} \right]^{\frac{1}{2}}. \tag{17}$$

Therefore

$$f(S, -S, S_{bz}) = (-1)^{S_b+S_{bz}} \Gamma_1 \frac{(S_a + S_b - S)!}{(S_a - S - S_{bz})!(S_b + S_{bz})!}, \tag{18}$$

where  $\Gamma_1 \equiv \left\{ \frac{(2S+1)!}{(S_{max}+S+1)!(S_{max}-S)!(S_{min}+S)!} \right\}^{1/2}$ . Thus

$$|S, -S\rangle = \Gamma_1 (a_\downarrow^\dagger)^{S+\frac{N_a-N_b}{2}} (b_\downarrow^\dagger)^{S-\frac{N_a-N_b}{2}} (a_\uparrow^\dagger b_\downarrow^\dagger - a_\downarrow^\dagger b_\uparrow^\dagger)^{\frac{N_a+N_b}{2}-S} |0\rangle. \tag{19}$$

Similarly, for  $S_z = S$ , we have

$$g(S, S, S_{bz}) = (-1)^{S_a-S+S_{bz}} \left[ \frac{(2S+1)!(S_a + S_b - S)!(S_a - S_{bz} + S)!(S_b + S_{bz})!}{(S_a + S_b + S + 1)!(S_a - S_b + S)!(S_a - S + S_{bz})!(S_b - S_{bz})!} \right]^{\frac{1}{2}}. \tag{20}$$

Therefore

$$f(S, S, S_{bz}) = (-1)^{S_a-S+S_{bz}} \Gamma_1 \frac{(S_a + S_b - S)!}{(S_a - S - S_{bz})!(S_b + S_{bz})!}. \tag{21}$$

Thus

$$|S, S\rangle = \Gamma_1 (a_\uparrow^\dagger)^{S+\frac{N_a-N_b}{2}} (b_\uparrow^\dagger)^{S-\frac{N_a-N_b}{2}} (a_\uparrow^\dagger b_\downarrow^\dagger - a_\downarrow^\dagger b_\uparrow^\dagger)^{\frac{N_a+N_b}{2}-S} |0\rangle. \tag{22}$$

It is clear that in  $|S, \pm S\rangle$ , there are  $\frac{N_a+N_b}{2} - S$  interspecies singlet pairs, plus  $S + \frac{N_a-N_b}{2}$   $a$ -atoms and  $S - \frac{N_a-N_b}{2}$   $b$ -atoms, each of which has  $z$ -component spin polarized as  $\pm 1$ . This is fully consistent with discussions in terms of the generating function method [22].

$$\mathbf{B.} \quad \left| \frac{N_a - N_b}{2}, S_z \right\rangle$$

For  $S = S_{min}$ , we have

$$g(S_{min}, S_z, S_{bz}) = (-1)^{S_{bz}} \left[ \frac{(2S_a - 2S_b + 1)!(2S_b)!(S_a + S_z - S_{bz})!(S_a - S_z + S_{bz})!}{(2S_a + 1)!(S_b + S_{bz})!(S_b - S_{bz})!(S_a - S_b + S_z)!(S_a - S_b - S_z)!} \right]^{\frac{1}{2}}. \quad (23)$$

Therefore

$$f(S_{min}, S_z, S_{bz}) = \Gamma_2 (-1)^{S_{bz}} \frac{(2S_b)!}{(S_b + S_{bz})!(S_b - S_{bz})!}, \quad (24)$$

where  $\Gamma_2 \equiv \left\{ \frac{(2S_a - 2S_b + 1)!}{(2S_a + 1)!(S_a - S_b + S_z)!(S_a - S_b - S_z)!(2S_b)!} \right\}^{1/2}$ . Thus

$$\left| \frac{N_a - N_b}{2}, S_z \right\rangle = \Gamma_2 (a_{\uparrow}^{\dagger})^{\frac{N_a - N_b}{2} + S_z} (a_{\downarrow}^{\dagger})^{\frac{N_a - N_b}{2} - S_z} (a_{\uparrow}^{\dagger} b_{\downarrow}^{\dagger} - a_{\downarrow}^{\dagger} b_{\uparrow}^{\dagger})^{N_b} |0\rangle, \quad (25)$$

as obtained in [19].

$$\mathbf{C.} \quad \left| \frac{N_a + N_b}{2}, S_z \right\rangle$$

For  $S = S_{max}$ , we have

$$g(S_{max}, S_z, S_{bz}) = \left\{ \frac{(2S_b)!(2S_a)!(S_a + S_b + S_z)!(S_a + S_b - S_z)!}{(2S_a + 2S_b)!(S_a + S_z - S_{bz})!(S_a - S_z + S_{bz})!(S_b + S_{bz})!(S_b - S_{bz})!} \right\}^{1/2}. \quad (26)$$

Therefore

$$\left| \frac{N_a + N_b}{2}, S_z \right\rangle = \Gamma_3 \sum_{S_{bz} = -S_b}^{S_b} c(S_{bz}) (a_{\uparrow}^{\dagger})^{S_a + S_z - S_{bz}} (a_{\downarrow}^{\dagger})^{S_a - S_z + S_{bz}} (b_{\uparrow}^{\dagger})^{S_b + S_{bz}} (b_{\downarrow}^{\dagger})^{S_b - S_{bz}} |0\rangle, \quad (27)$$

where  $\Gamma_3 = \left\{ \frac{(2S_b)!(2S_a)!(S_a + S_b + S_z)!(S_a + S_b - S_z)!}{(2S_a + 2S_b)!} \right\}^{1/2}$ , and  $c(S_{bz}) = [(S_a + S_z - S_{bz})!(S_a - S_z + S_{bz})!(S_b + S_{bz})!(S_b - S_{bz})!]^{-1}$ , which is nonzero only if the all the arguments of factorials are non-negative.

Especially, when  $S_z = \pm(S_a + S_b)$ , the state is a direct product of states of individual species.

$$\left| \frac{N_a + N_b}{2}, \pm \frac{N_a + N_b}{2} \right\rangle = \left| \frac{N_a}{2}, \pm \frac{N_a}{2} \right\rangle_a \left| \frac{N_b}{2}, \pm \frac{N_b}{2} \right\rangle_b, \quad (28)$$

where

$$\left| \frac{N_{\alpha}}{2}, \pm \frac{N_{\alpha}}{2} \right\rangle_{\alpha} = \frac{1}{\sqrt{N_{\alpha}!}} (\alpha_{\pm}^{\dagger})^{N_{\alpha}} |0\rangle, \quad (29)$$

with  $\alpha_{\pm}^{\dagger}$  representing  $\alpha_{\uparrow}^{\dagger}$  and  $\alpha_{\downarrow}^{\dagger}$ , is a ferromagnetic state of species  $\alpha$ .

#### IV. ENTANGLEMENT

In any state  $|S, S_z\rangle$ , the two species are entangled unless  $S = S_a + S_b$  and  $S_z = \pm S$ . In general, we can call a state polarized entangled BEC when  $S_z \neq 0$  and there is interspecies entanglement. For any state  $|S, S_z\rangle$ , we calculate the entanglement between the two species, which is quantified as the von Neumann entropy of the reduced density matrix of either species. One may con-

sider the entanglement between the occupation number of each of the four single-particle modes and the rest of the system [24]. Alternatively one simply considers the total the spins of the two species. Both approaches yield the same entanglement entropy  $\mathcal{E}$ ,

$$\mathcal{E} = - \sum_{m=-S_b}^{S_b} g^2(S, S_z, m) \log_{N_b+1} g^2(S_z, m). \quad (30)$$



The reason why both approaches lead to the same result, for any  $|S, S_z\rangle$ , is that the expansion is always automatically Schmidt decomposition with coefficients  $g(S, S_z, m)$ , no matter it is in terms of the spin basis states of the two species, as given in (13), or in terms of the occupation numbers of each species and each pseudospin state, as obtained by substituting (15) to (13).

In the following, we focus on the maximally polarized state  $|S, \pm S\rangle$ , because of the following reasons. First, most of our ground states are in this form. Second, in case the ground states are degenerate with respect to  $S_z$ , an infinitesimal symmetry breaking perturbation proportional to  $S_z$  picks out a maximally polarized state as the new ground state. Clearly, the entanglement entropies of  $|S, S\rangle$  and of  $|S, -S\rangle$  are equal, because  $g(S, m) = (-1)^{S_{\min}-S}g(-S, -m)$ .

For simplicity, we reduce our focus to the case of  $N_a = N_b = N$ , in which  $|S, -S\rangle = \Gamma_1(a_{\downarrow}^\dagger b_{\downarrow}^\dagger)^S(a_{\uparrow}^\dagger b_{\downarrow}^\dagger - a_{\downarrow}^\dagger b_{\uparrow}^\dagger)^{N-S}|0\rangle$  and  $|S, S\rangle = \Gamma_1(a_{\uparrow}^\dagger b_{\uparrow}^\dagger)^S(a_{\uparrow}^\dagger b_{\downarrow}^\dagger - a_{\downarrow}^\dagger b_{\uparrow}^\dagger)^{N-S}|0\rangle$ .

The calculation results are shown in FIG. 4 for four values of  $N$ . It can be seen that for a given  $N$ , entanglement always decreases when  $S$  increases.

We know

$$N_{\alpha\sigma} = N_\alpha/2 + \eta_\sigma S_{\alpha z}, \quad (31)$$

with  $\eta_\uparrow = 1$  and  $\eta_\downarrow = -1$ . Therefore, for any state, the

average number of  $\alpha$ -particles with spin  $\sigma$  is

$$\langle N_{\alpha\sigma} \rangle = \frac{N}{2} + \eta_\sigma M_{\alpha 1}, \quad (32)$$

where

$$M_{\alpha 1} \equiv \langle S_{\alpha z} \rangle, \quad (33)$$

Its fluctuation is

$$\Delta N_{\alpha\sigma} \equiv \sqrt{\langle N_{\alpha\sigma}^2 \rangle - (\langle N_{\alpha\sigma} \rangle)^2} = (M_{\alpha 2} - M_{\alpha 1}^2)^{1/2}, \quad (34)$$

where

$$M_{\alpha 2} \equiv \langle S_{\alpha z}^2 \rangle. \quad (35)$$

For  $|S, \eta_S S\rangle$ , with  $\eta_S = \pm 1$ , it is obtained that  $M_{a1} = M_{b1} = \eta_S \frac{S}{2}$ . Hence the total polarization is  $\eta_S S$ . It is also obtained that for this state,  $M_{a2} = M_{b2}$ , denoted as  $M_2$ , which depends on  $S$  and  $N$  in a more complicated manner, as shown in FIG. 5. For this state, one also has  $\Delta N_{a\uparrow} = \Delta N_{a\downarrow} = \Delta N_{b\uparrow} = \Delta N_{b\downarrow}$ , which is shown in FIG 6. One can see that the dependence of the fluctuation  $\Delta N_{\alpha\sigma}$  on  $S$  has a trend similar to the entanglement entropy. Indeed, the fluctuation  $\Delta N_{\alpha\sigma}$  is also a characterization of the interspecies entanglement [19].

Both  $M_{\alpha 1}$  and  $M_2$  enter the Gross-Pitaevskii-like equation governing the single-particle orbital wave function  $\phi_{\alpha\sigma}(\vec{r})$  under the ground state  $|S, \eta_S S\rangle$ , with  $S < N$ ,

$$\begin{aligned} & \left( \frac{N}{2} + \eta_\sigma \eta_S \frac{S}{2} \right) \left[ -\frac{\hbar^2}{2m_\alpha} \nabla^2 + U_{\alpha\sigma}(\mathbf{r}_\alpha) \right] \phi_{\alpha\sigma} + \left[ \frac{N^2}{4} + \eta_\sigma \eta_S \frac{(N-1)S}{2} + M_2 - \frac{N}{2} \right] g_{\sigma\sigma}^{(\alpha\alpha)} |\phi_{\alpha\sigma}|^2 \phi_{\alpha\sigma} \\ & + \left( \frac{N^2}{4} - M_2 \right) g_{\sigma\bar{\sigma}}^{(\alpha\alpha)} |\phi_{\alpha\bar{\sigma}}|^2 \phi_{\alpha\sigma} + \left( \frac{N^2}{4} + \eta_\sigma \eta_S \frac{NS}{2} + \frac{S^2}{2} - M_2 \right) g_{\sigma\sigma}^{(\alpha\beta)} |\phi_{\beta\sigma}|^2 \phi_{\alpha\sigma} + \left( \frac{N^2}{4} - \frac{S^2}{2} + M_2 \right) g_{\sigma\bar{\sigma}}^{(\alpha\beta)} |\phi_{\beta\bar{\sigma}}|^2 \phi_{\alpha\sigma} \\ & + g_e \left( M_2 - \frac{N^2}{4} - \frac{N}{2} + \frac{S}{2} \right) \phi_{\beta\bar{\sigma}}^* \phi_{\beta\sigma} \phi_{\alpha\bar{\sigma}} = \mu_{\alpha\sigma} \left( \frac{N}{2} + \eta_\sigma \eta_S \frac{S}{2} \right) \phi_{\alpha\sigma}. \end{aligned} \quad (36)$$

It is obtained by requiring the variation of the energy with respect to  $\phi_{\alpha\sigma}$  to be minimum, under the constraint  $\int |\phi_{\alpha\sigma}|^2 d\mathbf{r} = 1$ . Note that now the energy  $\langle \mathcal{H} \rangle$ , where  $\mathcal{H}$  is as given in (1), is treated as a functional of  $\phi_{\alpha\sigma}$ . The effective coefficients  $\epsilon_{\alpha\sigma}$  and  $K$ 's are now functionals of  $\phi_{\alpha\sigma}$ . In the limit  $S = 0$ , the equation reduces to that under the singlet ground state previously studied.

It can be seen that interspecies entanglement significantly affects the Gross-Pitaevskii equations, noting

$$M_2 = (\Delta N_{\alpha\sigma})^2 + S^2/4.$$

When  $S = N$ , the ground states  $|N, \eta_N N\rangle$  is disentangled between the two species, consequently there are only  $\phi_{\alpha\sigma}$  ( $\alpha = a, b$ ) with  $\sigma$  specified by  $\eta_\sigma \eta_N = 1$ . For  $|N, N\rangle = (1/N!) a_{\uparrow}^{\dagger N} b_{\uparrow}^{\dagger N} |0\rangle$ , there are only  $\phi_{a\uparrow}$  and  $\phi_{b\uparrow}$ . For  $|N, -N\rangle = (1/N!) a_{\downarrow}^{\dagger N} b_{\downarrow}^{\dagger N} |0\rangle$ , there are only  $\phi_{a\downarrow}$  and  $\phi_{b\downarrow}$ . For these two states,  $M_2 = N^2/4$ , and thus (36) reduces to

$$\left[ -\frac{\hbar^2}{2m_\alpha} \nabla^2 + U_{\alpha\sigma}(\vec{r}_\alpha) \right] \phi_{\alpha\sigma} + (N-1) g_{\sigma\sigma}^{(\alpha\alpha)} |\phi_{\alpha\sigma}|^2 \phi_{\alpha\sigma} + N g_{\sigma\sigma}^{(\alpha\beta)} |\phi_{\beta\sigma}|^2 \phi_{\alpha\sigma} = \mu_{\alpha\sigma} \phi_{\alpha\sigma}. \quad (37)$$

which is just Gross-Pitaevskii equations for the well stud-

ied two-component BEC.

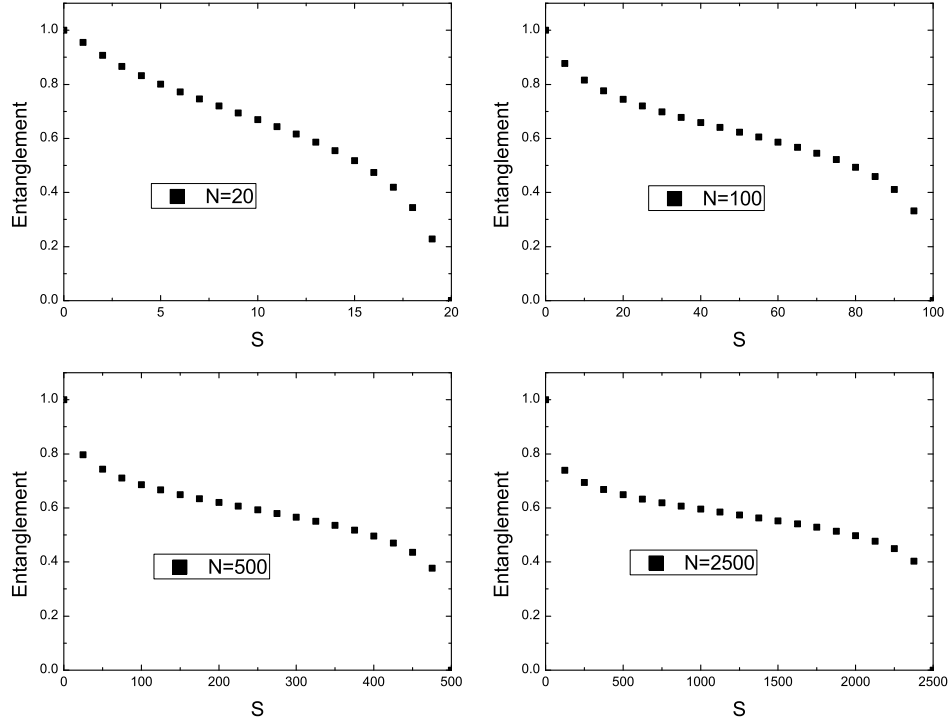


FIG. 4. Entanglement entropy of the interspecies entanglement in state  $|S, \pm S\rangle$ , with  $N_a = N_b = N$ , as a function of  $S$ .

## V. SUMMARY

To summarize, we have considered a more general case of the many-body Hamiltonian of a mixture of two species of pseudospin- $\frac{1}{2}$  bosons with interspecies spin-exchange interaction, with three effective parameters as given in (5). We have determined the ground states in all the regimes of these three parameters. Discontinuities of the ground states occur in some parameter boundaries. These are first order quantum phase transitions, as  $S^2$  or  $S_z$  have discontinuities in crossing the boundaries.

The two species are entangled in all the ground states except  $|\frac{N_a+N_b}{2}, \pm \frac{N_a+N_b}{2}\rangle$ , which is the ground states when  $K_e$  and  $C$  are both negative or sufficiently small positive, as shown in the phase diagrams. Very interestingly, when  $N_a = N_b$ , the ground state is the global singlet state  $|0, 0\rangle$  in the wide regime in which  $K_e$  is greater than the larger one between  $\frac{|B|-NC}{N+1}$  and  $|B|$ . This result confirms the previous arguments based on numerical estimation and perturbative analysis that the singlet ground state and the interspecies entanglement persist in a wide parameter regime [19, 20].

We have calculated the properties of  $|S, \pm S\rangle$  in details. For a given  $N$ , the polarization is equal to  $\pm S$ . The

entanglement decreases with as  $S$  increases. It reaches the maximal value 1 as  $S = 0$ , and reaches the minimal value 0 as  $S = N$ . The fluctuation of the particle number in either pseudospin state of each species has a similar behavior as the entanglement, reaching the maximal  $\sqrt{N(N+2)/12}$  as  $S = 0$  [19], and reaching the minimum 0 as  $S = N$ . The interspecies entanglement and polarization significantly affect the Gross-Pitaevskii equations governing the orbital wave functions associated with each pseudospin state of each species. This is a very interesting interplay between spin and orbital degrees of freedom. More phenomenology beyond that of the two-component BEC and can be experimentally observed is under investigation.

## Appendix A: $S^m$ and $S_z^m$ in all parameters regimes with $B \neq 0$

In this and next appendices, we find  $S^m$  in all regimes of the parameters. Neighboring regimes with a same ground state can be combined, as described in the main text. We consider  $B \neq 0$  in this Appendix.

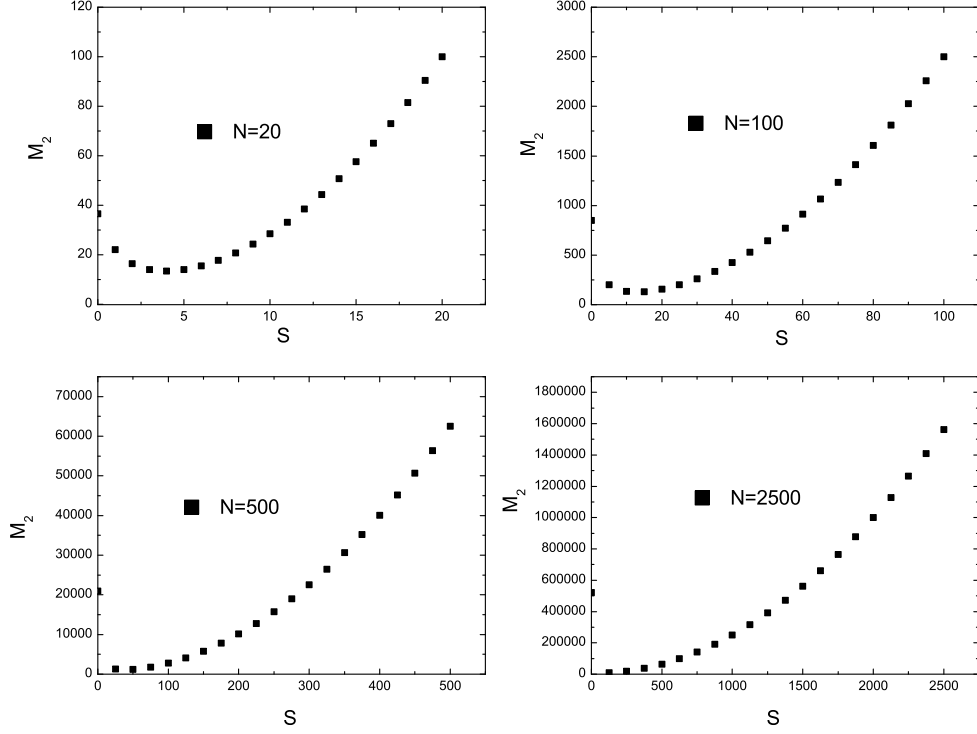


FIG. 5.  $M_2 \equiv \langle S_{\alpha z}^2 \rangle$ , for state  $|S, \pm S\rangle$ , as a function of  $S$ . Each plot is for a given  $N$  as indicated.

1.  $B \neq 0, C > 0$

Were there not be the constraint (10) on  $S_z$ , the minimum of the second term of (8) would be then at  $S_z = S_{z0}$ , where

$$S_{z0} \equiv \text{Int}(-B/2C)$$

is the integer closest to  $-B/2C$ . But one should, of course, consider the constraint (10), with the bounds  $\pm S$  determined by the sign of  $K_e$ .

a.  $B \neq 0, C > 0, K_e < 0$

Then  $S^m = S_{max}$ , under which  $S_z$  can vary in the largest possible range.  $S_z^m$  is determined by comparing  $S_{z0}$  with the bounds  $\pm S_{max}$ . If  $-S_{max} \leq S_{z0} \leq S_{max}$ , that is,  $C \geq \frac{|B|}{N_a + N_b}$ , then we have  $S_z^m = \text{Int}(-\frac{B}{2C})$ . If  $S_{z0} \leq -S_{max}$ , that is,  $C \leq \frac{B}{N_a + N_b}$ , then  $S_z^m = -S_{max}$ . If  $S_{z0} \geq S_{max}$ , that is,  $C \leq -\frac{B}{N_a + N_b}$ , then  $S_z^m = S_{max}$ .

b.  $B \neq 0, C > 0, K_e = 0$

Now there is no  $K_e$  term. However,  $-S_{max} \leq S \leq S_{max}$  is the largest possible range of  $S$ . If  $C \leq \frac{|B|}{N_a + N_b}$ , we have  $S_z^m = -\text{sgn}(B)S_{max}$ , which forces  $S^m = S_{max}$ . If  $\frac{|B|}{N_a + N_b} \leq C \leq \frac{|B|}{N_a - N_b}$ , then  $S_z^m = \text{Int}(-\frac{B}{2C})$  and thus  $|\text{Int}(-\frac{B}{2C})| \leq S^m \leq \frac{N_a + N_b}{2}$ . If  $C \geq \frac{|B|}{N_a - N_b}$ , then  $S_z^m = \text{Int}(-\frac{B}{2C})$  and  $\frac{N_a - N_b}{2} \leq S^m \leq \frac{N_a + N_b}{2}$ .

c.  $B \neq 0, C > 0, K_e > 0$

The minimum of the first term of (8) is at  $S = S_{min}$ , which constrains the range of  $S_z$ . As  $S_z$  term is positive,  $S^m$  may not be  $S_{min}$ . Nevertheless, if  $-S_{min} \leq S_{z0} \leq S_{min}$ , that is,  $C \geq \frac{|B|}{N_a - N_b}$ , then  $S^m = S_{min}$  and  $S_z^m = S_{z0}$ . If  $S_{z0} \leq -S_{min}$  or  $S_{z0} \geq S_{min}$ , that is, if  $C \leq \frac{|B|}{N_a - N_b}$ , then we have  $S_z^m = -\text{sgn}(B)S^m$ .

$S_m$  will be determined below altogether for various parameter regimes with  $S_z^m = -\text{sgn}(B)S^m$ . The present condition  $C > 0$  and  $K_e > 0$  overlaps only with the subcase  $K_e > -C$  in Appendix A 4. Hence there are three possibilities under the condition  $C \leq \frac{|B|}{N_a - N_b}$ .

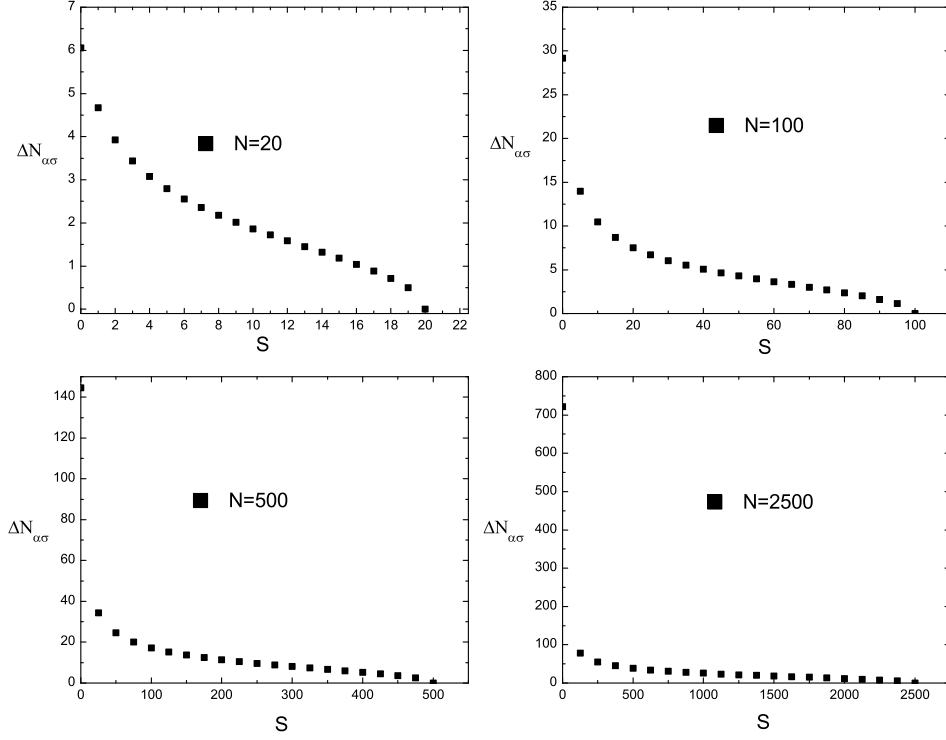


FIG. 6. The fluctuation  $\Delta N_{\alpha\sigma}$ , for state  $|S, \pm S\rangle$ , as a function of  $S$ . Each plot is for a given  $N$  as indicated.

## 2. $B \neq 0, C = 0$

In this case, in order that  $BS_z$  is smallest, we have  $S_z^m = -\text{sgn}(B)S^m$ , where  $\text{sgn}(B)$  represents the sign of  $B$ ,  $S^m$  is the value of  $S$  which minimizes  $E$ . Using the result of Appendix A 4, we know that there are three subcases. For  $K_e = 0$ ,  $S^m = S_{max}$ . For  $K_e > 0$ , the result of applies. For  $K_e < 0$ , the result of applies.

## 3. $B \neq 0, C < 0$

With  $C < 0$ , the  $S_z$ -dependent term in the energy (8) is minimized always at  $S_z^m = -\text{sgn}(B)S_m$ . This can be seen by representing this term as a parabola opening downward, with  $S_{z0}$  the maximal point. All three subcases of Appendix apply under the condition  $C < 0$ .

## 4. The cases with $B \neq 0$ and $S_z = -\text{sgn}(B)S$

As discussed above, for the case of  $B \neq 0$  and  $C \leq 0$ , as well as the case of  $B \neq 0, C > 0$  while  $K_e > 0$ , we have  $S_z = -\text{sgn}(B)S$ , therefore  $E$  can be expressed to

$$E = (K_e + C)S^2 + (K_e - |B|)S \quad (\text{A1})$$

$$= (K_e + C)(S - S_0)^2 + E_0'', \quad (\text{A2})$$

where

$$S_0 \equiv \frac{|B| - K_e}{2(K_e + C)}, \quad (\text{A3})$$

is the the extreme point of the parabola  $(K_e + C)(S - S_0)^2$ ,  $E_0''$  is independent of  $S$  and  $S_z$ .

### a. $K_e = -C$

This condition have overlap with  $C \leq 0$ , while do not overlaps with the condition  $C > 0$  and  $K_e > 0$ . Then  $E = (K_e - |B|)S + \text{const.}$  Therefore we know the following subcases, which .

If  $K_e = -C < |B|$ ,  $S^m = S_{max}$ .

If  $K_e = -C > |B|$ ,  $S^m = S_{min}$ .

If  $K_e = -C = |B|$ ,  $S^m$  is any any integer in the range  $S_{min} \leq S^m \leq S_{max}$ .

b.  $K_e > -C$

This condition overlaps with both the condition  $C \leq 0$  and the condition  $C > 0$  and  $K_e > 0$ .

Now that  $K_e + C > 0$ , the parabola  $(K_e + C)(S - S_0)^2$  open upwards. There are several subcases depending on the range of  $S_0$ , as one can conceive by considering the position of  $S_0$  related to the range (9). (i) If  $S_0 \leq S_{min}$ , which requires  $K_e \geq \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$ , then  $S^m = S_{min}$ . (ii) If  $S_{min} \leq S_0 \leq S_{max}$ , which requires  $\frac{|B|-(N_a+N_b)C}{N_a+N_b+1} \leq K_e \leq \frac{|B|-(N_a-N_b)C}{N_a-N_b+1}$ , which is a subset of  $-C < K_e < |B|$ , then  $S^m = S_0$ . (iii) If  $S_0 \geq S_{max}$ , which requires  $-C < K_e \leq \frac{|B|-(N_a+N_b)C}{N_a+N_b+1}$ , then  $S^m = S_{max}$ .

c.  $K_e < -C$

This condition overlaps with the condition  $C \leq 0$ , while do not overlap with the condition  $C > 0$  and  $K_e > 0$ .

With  $K_e + C < 0$ , the coefficient in (A2) is negative. The parabola  $(K_e + C)(S - S_0)^2$  open downwards.

We find that  $S^m = S_{max}$  for  $K_e < \frac{|B|-N_aC}{N_a+1}$ , while  $S^m = S_{min}$  for  $\frac{|B|-N_aC}{N_a+1} < K_e < -C$ , and  $S^m = S_{max}$  and  $S^m = S_{min}$  are two degenerate solutions for  $K_e < \frac{|B|-N_aC}{N_a+1}$ . This result is obtained by considering the position of  $S_0$  relative to the range (9), as the following. (i)  $S_0 < S_a$ , which requires  $K_e < \frac{|B|-N_aC}{N_a+1}$ , then  $S^m = S_{max}$ . (ii)  $S_0 = S_a$ , which requires  $K_e = \frac{|B|-N_aC}{N_a+1}$ , there are two degenerate solutions  $S^m = S_{max}$  and  $S^m = S_{min}$ . (iii) When  $S_0 > S_a$ , which requires  $K_e > \frac{|B|-N_aC}{N_a+1}$ , then  $S^m = S_{min}$ .

## Appendix B: $S^m$ and $S_z^m$ in all parameters regimes with $B = 0$

Now we look at the special situation of  $B = 0$ .

1.  $B = 0, C > 0$

Then  $S_z^m = 0$  in order to minimize  $CS_z^2$ . Subsequently, it is easy to see that  $S^m = S_{min}$  if  $K_e > 0$ ,  $S^m = S_{max}$  if  $K_e < 0$ , and  $S^m$  can be any legitimate  $S$ , i.e.  $S_{min} \leq S^m \leq S_{max}$ , if  $K_e = 0$ .

2.  $B = 0, C = 0$

There is no  $S_z$  term in  $E$ . Hence the values of  $S^m$  are the same for  $C > 0$ , while  $S_z^m$  can be any value in the legitimate ranges. If  $K_e > 0$ ,  $S^m = S_{min}$  while  $-S_{min} \leq S_z^m \leq S_{min}$ . If  $K_e < 0$ ,  $S^m = S_{max}$  while  $-S_{max} \leq S_z^m \leq S_{max}$ . If  $B = C = K_e = 0$ , then  $S_m$  and  $S_z^m$  are arbitrary values within the ranges (9) and (10).

3.  $B = 0, C < 0$

Then we have  $S_z = \pm S$  in order to minimize  $E$ , consequently  $E$  can be written as Equations (A1) and (A2), with  $B = 0$  and thus  $S_0 = -\frac{K_e}{2(K_e+C)}$ . The discussions in App. A 4 apply with  $B$  set to 0. But as  $B = 0$  causes both simplification and constraint. So we give details in the following.

a.  $B = 0, C < 0, K_e = -C$

Now  $E = K_e S + const.$  If  $K_e = -C < 0$ ,  $S^m = S_{max}$ ,  $S_z^m = \pm S_{max}$ . If  $K_e = -C > 0$ ,  $S^m = S_{min}$ ,  $S_z^m = \pm S_{min}$ .

b.  $B = 0, C < 0, K_e > -C$

Now that  $K_e + C > 0$ , the parabola  $(K_e + C)(S - S_0)^2$  open upwards. On the other hand now  $K_e > -C > 0$ , thus  $S_0 = -\frac{K_e}{K_e+C} < 0$ . Therefore  $S^m = S_{min}$ ,  $S_z^m = \pm S_{min}$ .

c.  $B = 0, C < 0, K_e < -C$

With  $K_e + C < 0$ , the parabola  $(K_e + C)(S - S_0)^2$  open downwards. We can directly use the result in App. A 4, setting  $B = 0$ , to know that  $S^m = S_{max}$  for  $K_e < -\frac{N_aC}{N_a+1}$ , while  $S^m = S_{min}$  for  $-\frac{N_aC}{N_a+1} < K_e < -C$ , and  $S^m = S_{max}$  and  $S^m = S_{min}$  are two degenerate solutions for  $K_e = -\frac{N_aC}{N_a+1}$ .

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[1] C. J. Pethick and H. Smith, *Bose-Einstein condensation in dilute gases* (Cambridge University Press, Cambridge,

2002).

- [2] T.-L. Ho, Phys. Rev. Lett. **81**, 742 (1998); T. Ohmi and K. Machida, J. Phys. Soc. Jpn. **67**, 1822 (1998).
- [3] C. K. Law, H. Pu, and N. P. Bigelow, Phys. Rev. Lett. **81**, 5257 (1998).
- [4] M. Koashi and M. Ueda, Phys. Rev. Lett. **84**, 1066 (2000);
- [5] T.L. Ho and S.K. Yip, Phys. Rev. Lett. **84**, 4031 (2000).
- [6] J. Stenger *et al.*, Nature **396**, 345 (1998); H.-J. Miesner *et al.*, Phys. Rev. Lett. **82**, 2228 (1999); D. M. Stamper-Kurn *et al.*, Phys. Rev. Lett. **83**, 661 (1999); H. Schmaljohann *et al.*, Phys. Rev. Lett. **92**, 040402 (2004).
- [7] S. Ashhab and C. Lobo, Phys. Rev. A **66**, 013609 (2002).
- [8] A. B. Kuklov and B.V. Svistunov, Phys. Rev. Lett. **89**, 170403 (2002).
- [9] S. Ashhab and A.J. Leggett, Phys. Rev. A **68**, 063612 (2003).
- [10] Z. B. Li and C. G. Bao, Phys. Rev. A **74**, 013606 (2006).
- [11] T. L. Ho and V. B. Shenoy, Phys. Rev. Lett. **77**, 3276 (1996).
- [12] H. Pu, and N. P. Bigelow, Phys. Rev. Lett. **80**, 1130 (1998).
- [13] P. Ao and S. T. Chui, J. Phys. B **33**, 535 (2000).
- [14] B. D. Esry *et al.*, Phys. Rev. Lett. **78**, 3594 (1997).
- [15] E. Timmermans, Phys. Rev. Lett. **81**, 5718 (1998).
- [16] M. Trippenbach *et al.*, J. Phys. B **33**, 4017 (2000).
- [17] C. J. Myatt *et al.*, Phys. Rev. Lett. **78**, 586 (1997); D. S. Hall *et al.*, Phys. Rev. Lett. **81**, 1539 (1998); G. Modugno *et al.*, Phys. Rev. Lett. **89**, 190404 (2002); G. Roati *et al.*, Phys. Rev. Lett. **99**, 010403 (2007); G. Thalhammer *et al.*, Phys. Rev. Lett. **100**, 210402 (2008); S. B. Papp, J. M. Pino and C. E. Wieman, Phys. Rev. Lett. **101**, 040402 (2008).
- [18] Y. Shi, Int. J. Mod. Phys. B **15**, 3007 (2001).
- [19] Y. Shi and Q. Niu, Phys. Rev. Lett. **96**, 140401 (2006).
- [20] Y. Shi, Europhys. Lett. **86**, 60008 (2009).
- [21] Y. Shi, Phys. Rev. A **82**, 013637 (2010).
- [22] Y. Shi, Phys. Rev. A **82**, 023603 (2010).
- [23] See, for example, A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Priceton University, Princeton, 1960).
- [24] Y. Shi, J. Phys. A **37**, 6807 (2004).